Neutron-induced reactions:

What it takes to do a Hauser-Feshbach calculation accurately

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University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. This work was supported in part from LDRD contract 00-ERD-028

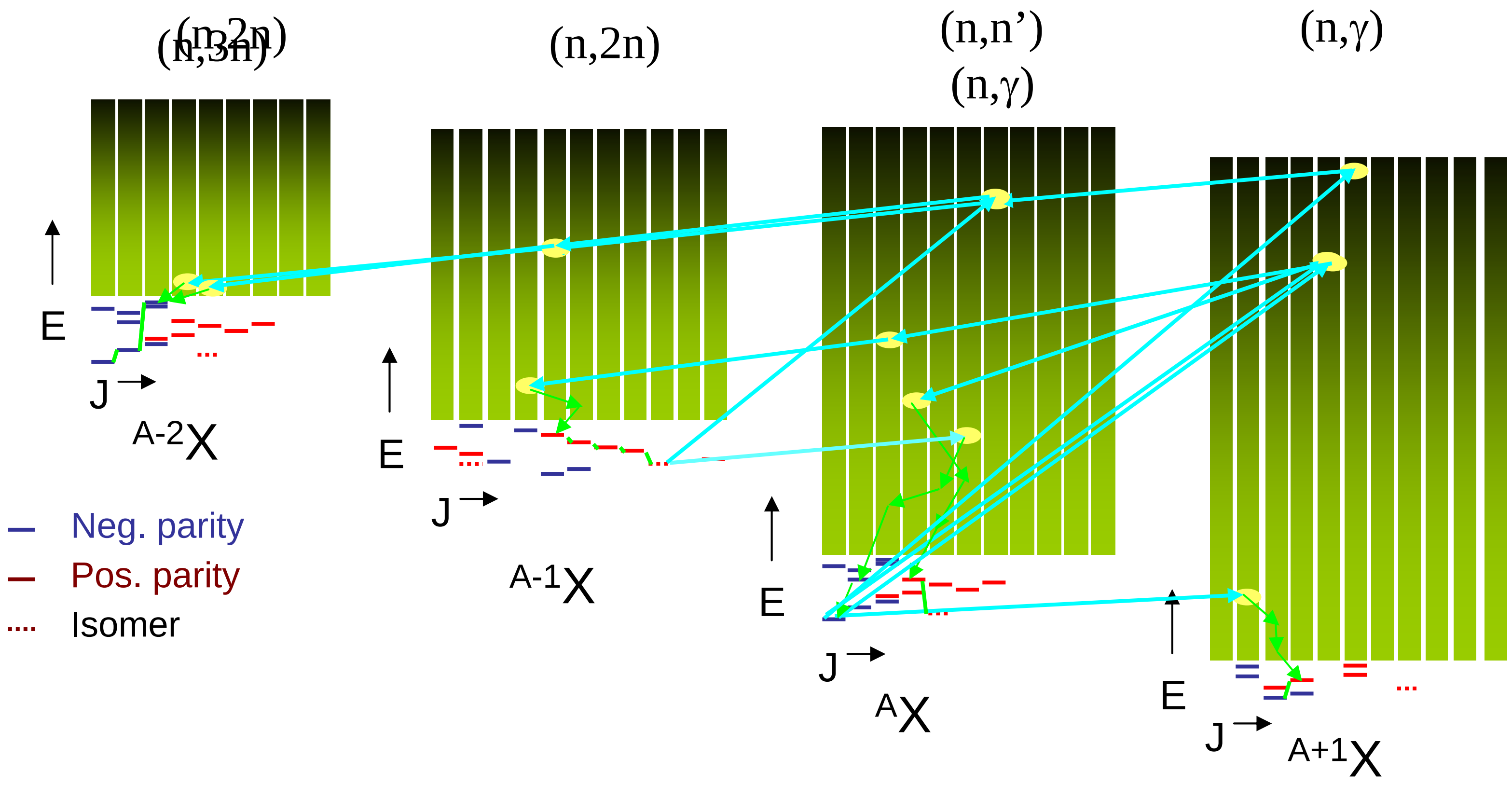
Goal: Accurate calculation for neutron-induced reactions on all target nuclei

- **Neutron-induced reactions are important for a wide range of processes**
  - Astrophysics
  - National security
  - Reactors
- **We need the ability to accurately predict a wide range of processes that can occur with neutron energies ranging from eV to 10-20 MeV**
  - Inelastic scattering - direct, compound, and pre-equilbrium
  - (n,2n)
  - (n,f)
- **Theory is needed when experiments can't be done, or a data is inadequate**
- **How accurate do we need the cross sections?**
  - It depends on what it is for
    - 1% to 20%

The Theory

- For most nuclei of interest here, i.e., intermediate to heavy near the valley of stability, we capture at E_x > 6 MeV into a region of high density with overlapping states
- Capture into fairly simple particle-hole excited states that are not eigenstates of the A+1 system
  - If the decay width of these states is smaller than their damping width, they will spread out into the large density of states in to form the so-called “compound nucleus”
    - Niels Bohr - The compound nucleus looses memory of how it was formed
    - Statistical decay: Hauser-Feshbach
  - Otherwise, they will decay via pre-equilibrium emission
    - Usually this starts to be important for E_n ~ 10 MeV
  - With a lower density, and for some low-lying states, we can have direct transitions, where structure actually matters

Example reaction networks



Hauser-Feshbach

- **Averaged cross section, can be derived under a set of assumptions**
- **The partial cross section for any channel process is**

$$\sigma_{cc'} = \sigma_c^{comp} \frac{\Gamma_{c'}}{\sum_{c''} \Gamma_{c''}}$$

$$\frac{d\sigma_{cc'}}{dE_{c'}} = \sum_{J,\Pi} \sigma_c^{comp} \frac{\sum_{l'} g_{l'J_{c'}} T_{l'}(E_{c'}) \rho(E_{c'}^{\max} - E_{c'})}{\sum_{c''l''} g_{l''J_{c''}} T_{l''}(E_{c''}) \int_o^{E_{c'}^{\max}} \rho(E_{c''}^{\max} - E_{c''}) dE_{c''}}$$

$$\sigma_c^{comp} = \frac{\pi}{k_c^2} \left\{ \sum_{s,l} g_J T_l(c) \right\} - \sigma_c^{preeq}$$

- **We need:**
  - **Transmission coefficients**
    - **Incident channel and all final states**
    - **Optical potential**
  - **Pre-equilibrium component**
  - **Gamma strength functions**
  - **Fission probabilities**
  - **Level densities**

Optical Potential

$$U(r) = V(r) + iW(r)$$

- Sets the scale of the reaction
  - Reaction cross section
    - The statistical processes take a fraction of the total reaction cross section - a piece of the pie so to speak
  - Also gives us the population of given J^{π} states
- Optical potentials are determined empirically by fitting to scattering data
  - Total cross section fairly well known
  - But usually not the reaction cross section
  - There are MANY optical potentials, which do you use
    - This is something of an art, so I usually go an ask Frank, or I use the recent global potential of Koning & Delaroche
    - Typically, 5-10% uncertainty - but can we quantify it?
  - We need a more fundamental and microscopic theory
  - In principle, the optical potential can be computed from DFT with an appropriate effective interaction
    - HARD! - SciDAC proposal seeks to address this issue

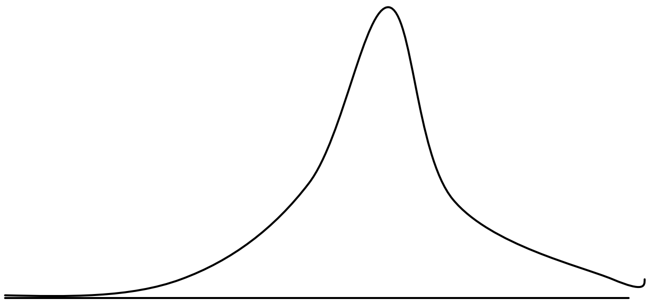
$$\langle \chi_k | U_{HF} | \chi_k \rangle + \sum_{RPA} \langle \chi_{k'} \psi_f^A | V | RPA_{A+1}^{2p-1h} \rangle \frac{1}{E - E_{RPA} + i\varepsilon} \langle RPA_{A+1}^{2p-1h} | V | \psi_i^A \chi_k \rangle$$

Pre-equilibrium processes

- Formation of the compound nucleus is a multi-step process
- Remember the initial states damp into the compound
- If the width for neutron emission is comparable to the damping width, the state can decay prior to formation of the compound nucleus
- Models:
- Exciton - coupling to particle hole states, and their densities
  - A bit primitive
    - Empirical matrix element, so it doesn't have solid predictability
    - Angular momentum transfer is not correct - usually assumes compound - this can affect several decay processes
- Feshbach-Koonin-Kermin
  - Microscopic foundation - questions of getting it right
  - Substantially more difficult, it needs better structure input
  - An extension of microscopic theories for the optical potential
  - Computationally demanding

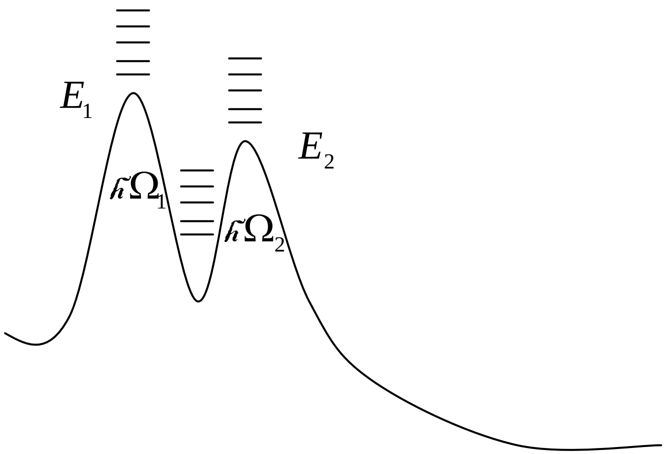
Gamma-strength function

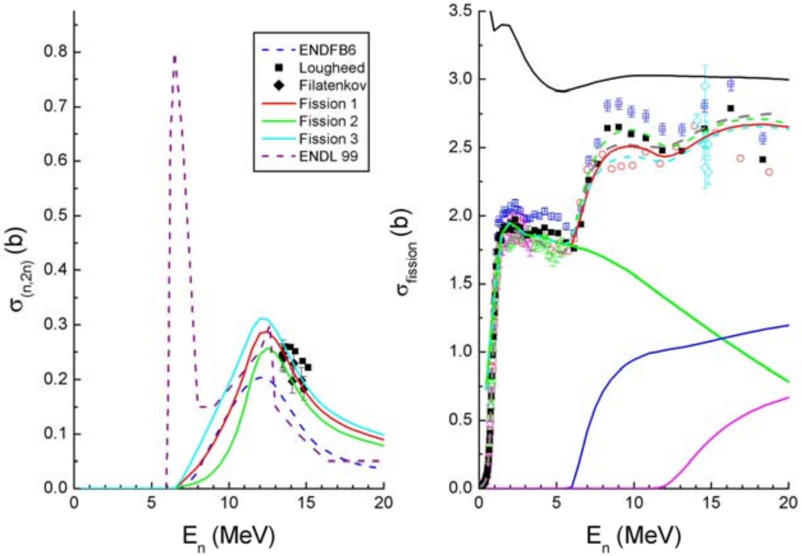
- **Important for (n,γ)**
- **Radiation widths known for stable targets**
- **E1 is a dominant component because of phase space**
  - **BR ~ E_γ^3**
  - **Lorentzian? pygmy?**
- **Also M1 and E2**
- **Transition from continuous level density to discrete states, where explicit structure matters**
  - **Are there conservation rules, like K-quantum number**
    - **Affects isomer production and possibly fission**
- **Computationally demanding - AFMC**



Fission

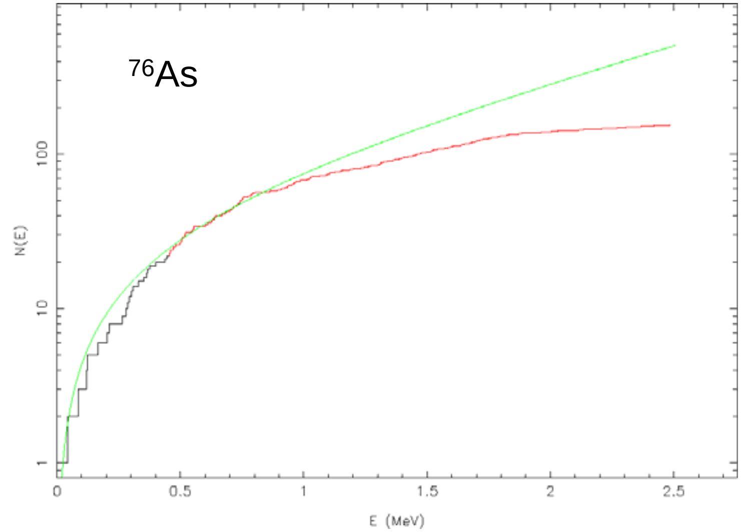
- **Very important for AFC and national security applications**
- **Fission probabilities affect other processes, e.g., (n,2n)**
- **No predictive theory of fission really exists today**
- **Generally, a barrier penetration model is used**
  - **Bjornholm & Lynn; Nix; Britt**
  - **Depends on Barriers, curvatures wi an inertial parameter, and density o states above the barrier**
  - **Empirical, and HIGHLY uncertain without data to fit parameters to**
- **We need a predictive model for fission - VERY HARD!**

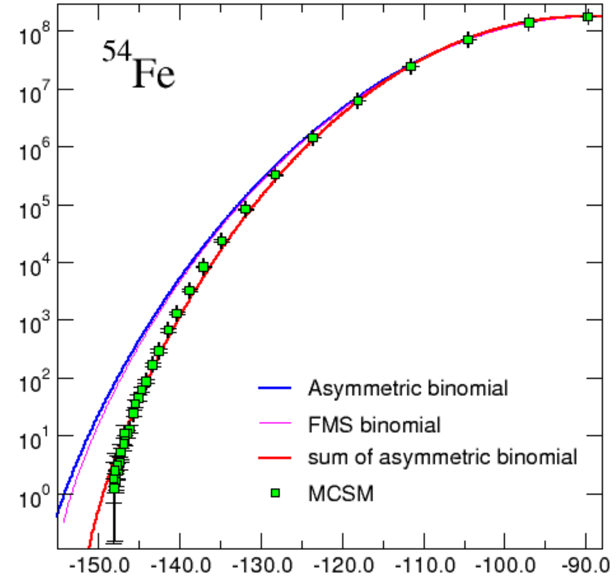




Level densities

- **Important because it is exponentially growing, thus phase space rules**
- **Tends to help determine threshold behaviors, as in (n,2n), also (n,γ)**
- **How accurately do we know it?**
  - **D_0 resonance spacings on stable nuclei**
  - **Discrete levels at low excitation energy**
  - **Gilbert-Cameron - Back-shifted Fermi gas**
  - **Better microscopic theories are needed**
    - **Moments and AFMC**
    - **Computationally demanding**





Summary

- **Hauser-Feshbach, or statistical decay, is fairly straight forward and is reasonably grounded in physics**
  - **Conceptually easy to do**
- **But, it has many components for the decay channels, each of which are a separate, and computationally demanding challenge**
  - **Optical potential, pre-equilibrium emission, γ Strength functions, fission probabilities, level densities**
  - **Classic example of GARBAGE IN - GARBAGE OUT**

A lot of work needs to be done to put each of the components of HF on a solid microscopic foundation that will permit accurate and reliable calculations of neutron-induced reactions relevant to Astrophysics, Stockpile Stewardship, and AFC